Raul Garcia-Patron
Petros Wallden
Milos Prokop

Tutorial 7

IQC 2023-24
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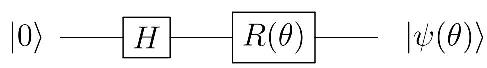
Problem 1

Consider a 2-dimensional Hamiltonian $\mathcal{H}$ where $|+_{\frac{\pi}{4}}\rangle$ is the eigenvector with 0 eigenvalue and $|-_{\frac{\pi}{4}}\rangle$ is the other eigenvector with eigenvalue 1. Recall that you can always write an operator as the sum (taken over different eigenvalues) of the product of the eigenvalue with the projection to the corresponding eigenspace.

a. Write the Hamiltonian in terms of the eigenvectors and in matrix form (in the computational basis).

b. Express $\mathcal{H} = \sum_i c_i P_i$ in terms of Pauli matrices ($P_i \in \{I, X, Y, Z\}$) using the formula for calculating the coefficients c_i given in the lecture, and for simplicity here too: $c_i = \langle P_i, \mathcal{H}\rangle$, where $\langle A, B\rangle := \frac{Tr(A^\dagger B)}{2}$.

c. Evaluate the output state $|\psi(\theta)\rangle$ given by the following parametrised circuit :



d. For any state express $E(\theta) := \langle\psi(\theta)| \mathcal{H} |\psi(\theta)\rangle$ by using part b, in terms of $\langle\psi(\theta)| P_i |\psi(\theta)\rangle$.

e. Now find the ground state with the following steps:

- Start from $\theta_0 = 0$
- Estimate the gradient in each step using $\Delta(\theta_i) = E(\theta_i + \delta\theta) - E(\theta_i - \delta\theta)$ where $\delta\theta = \frac{\pi}{8}$
- Update θ accordingly by moving in the opposite direction of the gradient by a step $\delta\theta$, i.e. set $\theta_1 = \theta_0 \pm \delta\theta$ with the sign determined by the computed gradient
- Continue this for another two steps and find the value of θ which minimises $\langle\mathcal{H}\rangle$.

Problem 2

Consider the cost function of a Binary Optimisation problem with up to cubic terms:

$$C(x) = \sum_i a_i x_i + \sum_{i,j} b_{ij} x_i x_j + \sum_{i,j,k} c_{ijk} x_i x_j x_k$$

Each of the x_i is a binary variable $x_i \in \{0, 1\}$, and the index i runs from 1 to n. Finding the configuration with the smallest cost gives a general cubic, n-binary variables optimisation problem. For a number of reasons, one may be interested in turning this problem to Quadratic Unconstrained Binary Optimisation (QUBO) problem, i.e. restricting the cost function to a cost function that has at most quadratic terms (but no cubic terms).

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a. Let $g(x,y) := (2 - x_i - x_j - x_k)y = 2y - x_i y - x_j y - x_k y$, where $y \in \{0,1\}$ is another, new, binary variable. Show that the following functions are the same:

$$\begin{aligned} f(x) &= -x_i x_j x_k \\ &= \min_y g(x,y) \end{aligned}$$

This proves that we can replace cubic terms $-x_i x_j x_k$ with quadratic ones $(2 - x_i - x_j - x_k)y$ with the cost of introducing (in this case a single) extra variable y. Note, that we are interested in the minimum value of the cost function (i.e. we are taking the minimum of this expression over all binary variables, including the newly introduced y).

b. Find how we reduce the order of a cost function that has fourth order terms of the form $x_i x_j x_k x_l$ and make it quadratics (i.e. an expression with at most quadratic terms).

c. Consider the cost function:

$$C(x) = -5x_1 x_2 x_3 x_4 + x_2 + 2x_3$$

Using the result of b. reduce the order to quadratic. Then change the variables to spins using this $x_i = \frac{1-s_i}{2}$. Construct a Hamiltonian $\mathcal{H}_C$ by replacing each spin variable s_i with the Pauli Z_i gate. Finally, calculate the expectation value $\langle\psi| \mathcal{H}_C |\psi\rangle$ of the state $|\psi\rangle$ if $|\psi\rangle = a\,|00000\rangle + b\,|01011\rangle$ where the last qubit denotes the extra qubit, i.e. $|s_1 s_2 s_3 s_4 y\rangle$.